Can low-frequency breathers exist in a quasi-1D crystal?

A. V. Savin[1], E. A. Zubova[1], L. I. Manevitch[1]

[1] *Institute of Chemical Physics RAS, 4 Kosygin str., Moscow 119991, Russia*

We investigate a quasi-1D crystal: 2D system of coupled linear chains of particles with strong intra-chain and weak inter-chain interactions. Nonlinear dynamics of one of these chains when the rest of them are fixed is reduced to the well known Frenkel-Kontorova (FK) model. Its continuum limit, sine-Gordon (sG) equation, predicts two types of soliton solutions: topological solitons and breathers. It is known that the quasi-1D topological solitons exist also in a 2D system of coupled chains and even in a 3D model of a polymer crystal. Numerical simulation shows that the breathers inherent to the FK model do not exist in the system of chains. The effect changes scenario of kink-antikink collision at small velocities: it always results only in intensive phonon radiation while kink-antikink recombination in the FK model results in long-living low-frequency sG breather creation. The reason of the difference is that the model of coupled chains catches 'acoustic' part of phonon spectrum of a crystal while the FK model does not. Low-frequency SG breathers in a crystal intensively emit resonant 'acoustic' phonons and come to ruin.

The Frenkel-Kontorova (FK) model (a linear chain of harmonically coupled particles on the sine substrate) [1] is the the most commonly used and comprehensively investigated (see monographs [2, 3]) 1D model of a crystal. In the case of weak substrate potential (weakly discrete system) it seems to be especially appropriate for polymer crystals: quasi-1D topological soliton-like excitations predicted by its continuum limit, sine-Gordon (sG) equation, exist in a 2D system of coupled chains [4, 5] and even in a 3D model of a polymer crystal (see, for example, [6]). SG equation is the only nonlinear wave equation of type

$$u_{tt} - u_{xx} + g(u) = 0 \qquad (1)$$

which possesses also one-parametric family of exact solutions in the form of low-frequency breathers [7]. Frequencies of the breathers fill the gap between zero and the minimal frequency in phonon spectrum $\Omega_{FK}(0)$. If the breather frequency approaches $\Omega_{FK}(0)$, the breather amplitude tends to zero, and the breather width – to infinity ('phonon' limit). If the breather frequency tends to zero, the breather approaches a full kink-antikink profile.

Numerical simulations [8, 9] show that in the FK model the sG breathers survive, and, although lose the energy due to resonances of odd multiples to the breather frequency with phonon frequencies, have their lifetime long enough even in the case of strong discreteness (more than hundred periods when the third harmonic to its frequency becomes higher than the upper phonon band edge [8]). In the case of weak discreteness losses of energy are hardly perceptible [9].

In connection with studying real physical quasi-1D systems such as long Josephson junctions and quasi-1D ferromagnets there emerged many works treating behavior of sG breathers under action of perturbations breaking exact integrability: dissipative and diverse conservative terms (see [10, 11], and [12] and references therein). Analytical treatment of the problem is possible as perturbation in the inverse scattering transform [10] or as multiple-scale asymptotic expansion [11] in the limit of high breather frequencies, and one can obtain some estimates in general case [12]. As one can easily predict, the breather lifetime proved to be long if perturbation is small.

In nonintegrable models with substrate potentials sufficiently different from the sine function breather-like long-living nonlinear excitations are observed numerically (ϕ^4 - [13], double sG, square well potential - [14]). For the ϕ^4 model it is shown [15] that the radiation rate of a small-amplitude 'breather' lies beyond all orders in asymptotic expansion.

All this allows one to look on such breathers as being 'elementary excitations' in a crystal, together with kinks and antikins (topological solitons) and phonons. This implies that the breathers can noticeably contribute to thermodynamic properties of a crystal [16] and even must be used in phenomenological approaches to sG thermodynamics instead of phonons [17, 18]. We show that this conclusion based on analysis of the FK model (a chain on a substrate) is not valid for a more realistic model of a crystal: a system of coupled chains.

Let us take a system of coupled linear chains of (classical) particles (fig.1). To catch the main physical meaning of the model it is enough to allow inter-chain interactions only between particles of the nearest neighboring chains. Then Hamiltonian of the system is written as

$$H = \sum_{m,n}\{\frac{1}{2}\dot{u}_{m,n}^2 + \frac{1}{2}(u_{m,n+1} - u_{m,n} + c - c_0)^2$$
$$+ \sum_{j=-\infty}^{+\infty} U(r_{m,n;j})\}, \qquad (2)$$

where the dot denotes time derivative, c_0 is the period of a separate chain, c - the longitudinal period of the crystal, $u_{m,n}$ is longitudinal deviation of the particle (m, n) from its equilibrium position (shown in fig.1) in the crystal (we keep transversal deviation $y_{m,n} = 0$), the potential $U(r_{m,n;j})$ describes interaction of the n-th particle in the m-th chain with the $(n+j)$-th particle in the $(m + 1)$-th chain, $r_{m,n;j}$ being the distance between the particles

$$r_{m,n;j} = \{[(j - (-1)^m/2)c + u_{m+1,n+j} - u_{m,n}]^2 + b^2\}^{1/2}.$$

The ground state of the system ($u_{m,n} = \dot{u}_{m,n} = 0$) has the
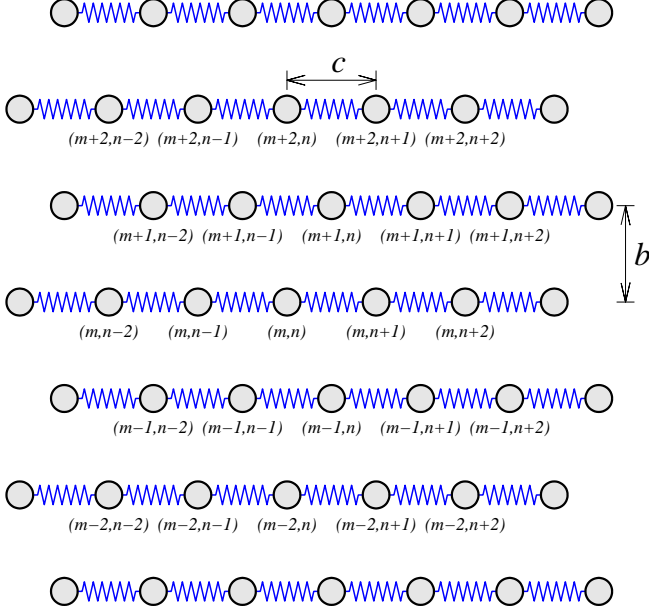
FIG. 1: 2D model of quasi-1D system: intra-chain interactions are much stronger than inter-chain ones (weak discreteness limit). We choose unit length so that $c = 1$ in the equilibrium ground state of the crystal.

energy per particle

$$E(b, c, c_0) = (c - c_0)^2 + \sum_{j=-\infty}^{+\infty} U(R_j),$$

where $R_j = [b^2 + c^2(j+1/2)^2]^{1/2}$ is the distance between the n-th and the $(n + j)$-th particles of the m-th (m is odd) and $(m+1)$-th chains. Equilibrium values of b and c minimize the expression at given c_0. Equivalently, if one chooses c as unit length, one can find equilibrium values of c_0 and b. Hereafter we imply that the crystal is initially in its equilibrium ground state with $c = 1$.

The present 2D model of quasi-1D crystal was first introduced in [4]. One can take into account also transversal displacements of particles [5]. The model allows existence and propagation of quasi-1D topological soliton-like excitations. In [4, 5] have been used the Morse potential of particle interactions $U(r_{m,n;j})$ as very suitable for numerical calculations. Here we exploit the more physical Lennard-Jones potential (truncated):

$$U(r) = \varepsilon \left(\frac{r_0}{r}\right)^6 \left[\left(\frac{r_0}{r}\right)^6 - 2\right] f(r) \qquad (3)$$

where the truncation function $f(r) = \{1 - \tanh[\mu(r-d_0)]\}/2$ ($\mu \sim 1$, $d_0 \gg r_0$) is introduced for convenience of numerical calculations. It allows one to avoid taking into account interactions of the particles placed one from another farther than $r \approx d_0$.
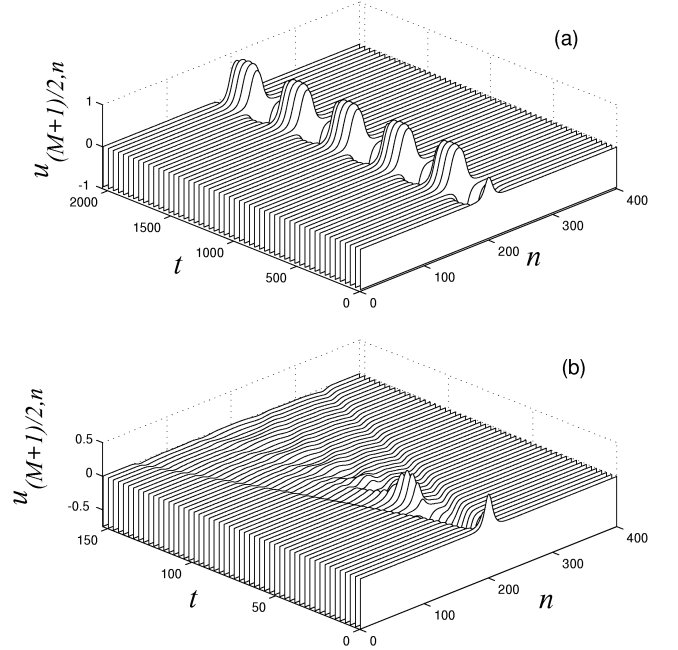

FIG. 2: Low-frequency sG breather in the crystal ($\epsilon = 0.007$, $M = 51$, $N = 400$): oscillations in the FK model (the case of immobile neighboring chains) (a) and degradation in the full model of interacting mobile chains (b). We show the displacements $u_{26,n}$ of the 26th chain containing the breather in successive time moments t. Breather frequency is $\omega_b = 0.0157$.

It is known [19] that if the equilibrium distance between particles r_0 falls into the interval $0.91 < r_0 < \infty$ shape of the substrate potential is close to the sine function. We have chosen $r_0 = 1.67$ ($d_0 = 20$, $\mu = 2$) because it corresponds to model of polyethylene crystal with 'united atoms' [6, 20]. At this value of r_0 the substrate generated by immobile neighbors

$$V(u) = 2 \sum_{j=-\infty}^{+\infty} [U(r_j(u)) - U(R_j)], \qquad (4)$$

where $r_j(u) = [b^2 + (u + j + 1/2)^2]^{1/2}$ (note that $R_j = r_j(0)$), is the sine function accurate within 0.1%: $V(u) \simeq \epsilon[1 - cos(2\pi u)]$, where substrate amplitude $\epsilon = 0.1757\varepsilon$. So dynamics of one chain when the rest of them are fixed is reduced to the well known FK model:

$$H_{FK} = \sum_n \{\frac{1}{2}\dot{u}_n^2 + \frac{1}{2}(u_{n+1} - u_n)^2 + V(u_n)\}. \qquad (5)$$

The width of a static kink in the model of polyethylene crystal with 'united atoms' (about 30 periods) coincides with the width of a static kink in our model of coupled chains if the intensity of inter-chain interactions $\varepsilon = 0.0007$. We have also considered the cases of stronger interactions $\varepsilon = 0.007$, 0.07. The first two cases correspond to limit of weak discreteness. In the last case the sound velocity in transversal direction is

equal to one in longitudinal direction (see table I). When the chains are assembled into the crystal the transversal equilibrium period appears to be $b = 1.5666$ independent on ε. Only c_0 is ε-dependent.

The system of equations of motion for the quasi-1D crystal takes the form:

$$\ddot{u}_{m,n} = -\frac{\partial H}{\partial u_{m,n}}, \qquad (6)$$
$$n = 0, \pm 1, \pm 2, ..., \quad m = 0, \pm 1, \pm 2, ...$$

with the Hamiltonian (2). In numerical simulations we considered the dynamics of a bounded rectangular fragment of the crystal ($1 \le n \le N$, $1 \le m \le M$) with fixed boundary conditions in both directions.

We have compared behavior of a sG breather in the FK model (all the chains are kept immobile except one - with number $m = (M+1)/2$ - containing the breather) and in the model of coupled chains (all the chains are mobile).

Numerical simulation shows that the breather in the FK model enjoys regular stable oscillations for a very long time (fig.2 (a)). The situation changes drastically if we allow all the chains in the crystal to move. The breather quickly comes to ruin. Its lifetime is less than two its periods (fig.2 (b)). The effect is observed by all three values of the inter-chain interactions $\varepsilon = 0.07, 0.007, 0.0007$. The destruction results from the intensive emission of phonons into the neighboring chains (see fig.3). Energy of the breather spreads to all the particles. So one can conclude that the low-frequency sG breathers are absent in the model of coupled chains.

With this in mind, one can suppose the difference between the two models under study in scenario of kink-antikink recombination when they collide with small velocities. Indeed, in the FK model (with the sine potential as well as with the double sine or square well ones) kink and antikink can form oscillating breather-like state, their energy remaining for a long time localized [14] – see fig. 4 (a), while in the model of coupled chains their energy scatters at ones with phonons – see fig.4 (b).

The reason of the effect observed seems to be that the two models of a crystal possess qualitatively different phonon spectra. Namely, the FK model has a gap between $\omega = 0$ and the lower edge of the spectrum $\Omega_{FK}(0)$ while in the model of coupled chains - like in a genuine crystal - the minimal possible frequency is $\omega_{min} = 0$. Let us show it. As we have chosen particles numeration not coinciding with one based on translation of the crystal cell, phonon modes have the more
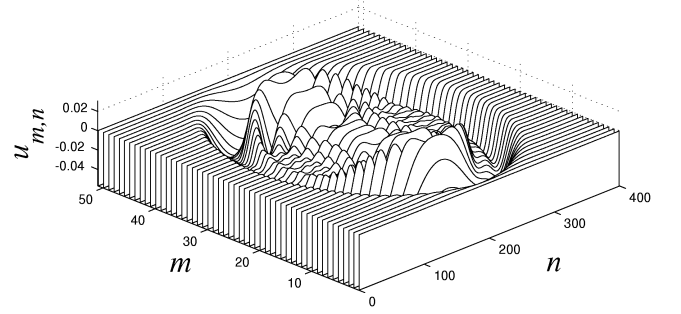

FIG. 3: State of the crystal ($M = 51$, $N = 400$) of coupled chains ($\epsilon = 0.007$) resulting from destruction of low-frequency ($\omega_b = 0.0157$) sG breather placed onto the 26th chain. The displacements $u_{m,n}$ are shown in the time moment $t = 150$.
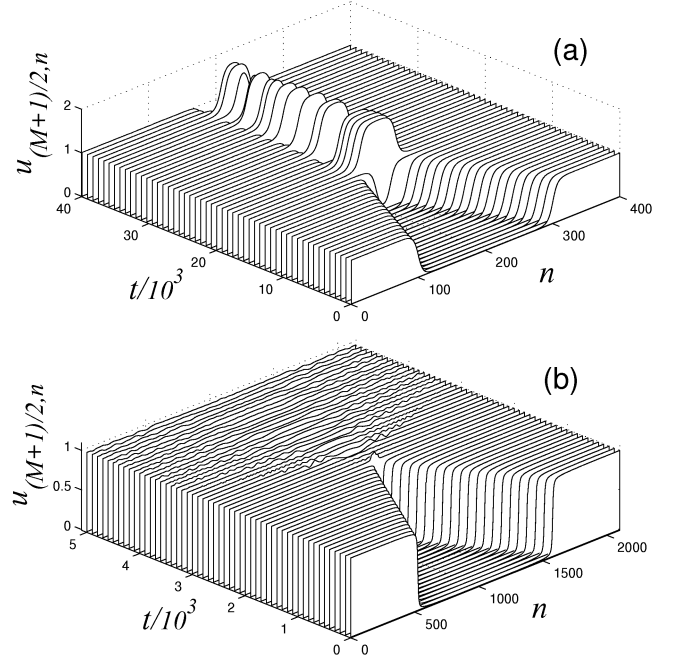

FIG. 4: Kink-antikink recombination in a chain of the crystal ($\varepsilon = 0.007$) having immobile (a) and mobile (b) neighboring chains. Collision of solitons in the FK model (soliton velocity $s = 0.005$) results in creation of a low-frequency sG breather. Collision of solitons in the model of all moving chains (soliton velocity $s = 0.25$) results in intensive radiation of phonons.

complicated form:

$$u_{2m,n} = A \exp i[q_1 n + q_2 2m - \omega t],$$
$$u_{2m+1,n} = A \exp i[q_1(n - 1/2) + q_2(2m+1) - \omega t], \quad (7)$$
$$n = 0, \pm 1, \pm 2, ..., \quad m = 0, \pm 1, \pm 2, ...$$

where $A \ll 1$, and q_1, $q_2 \in [0, \pi]$. Substituting the anzatz (7) into the linearized system of equations (6) with imposed periodic boundary conditions in both directions one can obtain

TABLE I: Dependence of the longitudinal s_x and transversal s_y sound velocities, characteristic frequencies ω_{max} and $\Omega_{FK}(0)$ on the value of the parameter ε.

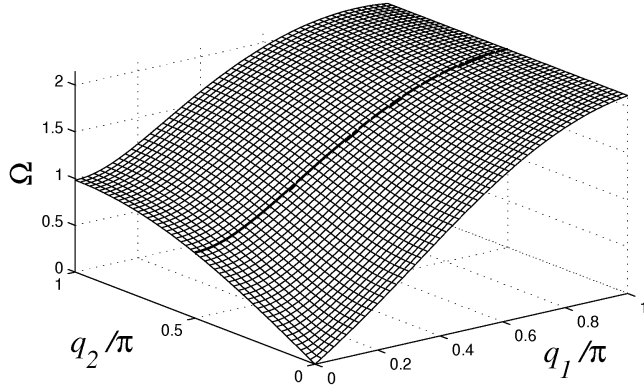| ε	s_x	s_y/b	ω_{max}	$\Omega_{FK}(0)$
0.07	0.7530	0.4916	2.1174	0.6952
0.007	0.9781	0.1555	2.0120	0.2197
0.0007	0.9978	0.0492	2.0012	0.0694

FIG. 5: Dispersion surface $\omega = \Omega(q_1, q_2)$ for the model of coupled chains. The model parameters $r_0 = 1.67$, $\varepsilon = 0.07$. The curve on the surface is the dispersion curve for corresponding FK model (approximation of immobile chains) $\omega = \Omega(q_1, \pi/2)$.

the dispersion equation

$$\Omega(q_1, q_2) = \{2(1 - \cos q_1)$$
$$+4\sum_{j=0}^{+\infty} K_j[1 - \cos((j+1/2)q_1)\cos q_2]\}^{1/2}, \quad (8)$$

where rigidities are $K_j = U''(R_j)(j + 1/2)^2/R_j^2 + U'(R_j)b^2/R_j^3$. Values of the rigidities are in direct proportion to the parameter of inter-chain interation ε; for $\varepsilon = 0.07$ they are $K_0 = 0.199$, $K_1 = -0.061$, $K_2 = -0.014$, $K_3 = -0.002$. We have presented the plot of the dispersion surface for $\varepsilon = 0.07$ in fig.5 together with the dispersion curve for the corresponding FK model.

Dispersion equation (8) gives the minimal $\omega_{min} = \Omega(0, 0) = 0$ and the maximal

$$\omega_{max} \equiv \Omega(\pi, q_2) = 2(1 + \sum_{j=0}^{+\infty} K_j)^{1/2}$$

possible frequencies, the velocity of longitudinal long phonons

$$s_x = \lim_{q_1 \to 0} \Omega(q_1, 0)/q_1 = [1 + \sum_{j=-\infty}^{+\infty} (j+1/2)^2 K_j]^{1/2},$$

and the velocity of transversal long phonons

$$s_y = b \lim_{q_2 \to 0} \Omega(0, q_2)/q_2 = b(\sum_{j=-\infty}^{+\infty} K_j)^{1/2}.$$

The cut of the dispersion surface (8) at $q_2 = \pi/2$ produces the dispersion curve for the corresponding FK model:

$$\Omega_{FK}(q) = \Omega(q, \pi/2) = \{2[1 - \cos(q)] + 2\sum_{j=-\infty}^{+\infty} K_j\}^{1/2}.$$

Now the minimal frequency is $\Omega_{FK}(0) = (2\sum_j K_j)^{1/2} > 0$. Dependence of the velocities s_x, s_y, and the frequencies ω_{max} and $\Omega_{FK}(0)$ on the parameter of inter-chain interactions ε is presented in the Table I.

So, with such a phonon spectrum, the model of interacting chains can not possess even approximate low-frequency breather solutions. Their frequencies fall into phonon band, the resonance interaction between a breather and a phonon takes place and the breather energy is transmitted to the phonons, resulting in quick breather degradation. And evidently it is the case in real (for example, polymer) crystals.

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